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FILE COVERS 1907 - 10 Nov 2004  VOL 141 ISS 20
FILE LAST UPDATED: 9 Nov 2004  (20041109/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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L3                STR
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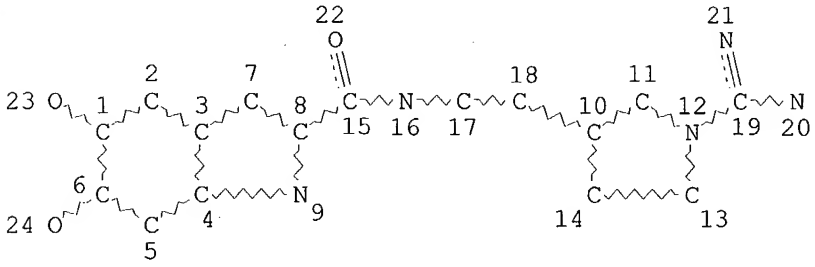


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  24

STEREO ATTRIBUTES: NONE
L5             8 SEA FILE=REGISTRY SSS FUL L3
L6             5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5


=>
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=> d ibib abs hitstr 16 1-5

L6   ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2004 ACS on STN
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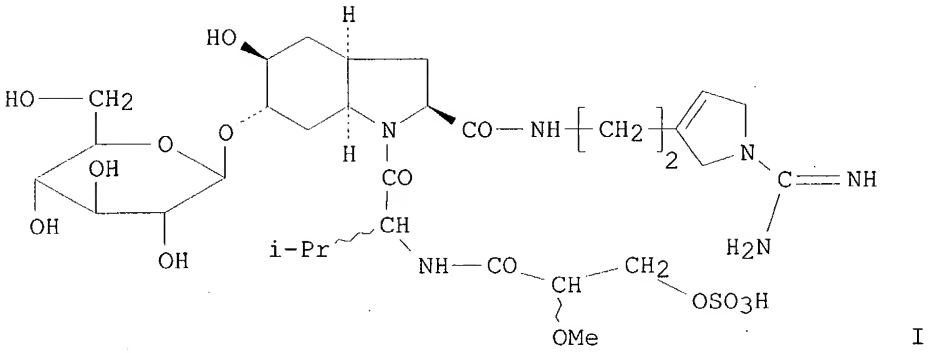
ACCESSION NUMBER: 2004:553526 HCAPLUS
DOCUMENT NUMBER: 141:221980
TITLE: Dysinosins B-D, inhibitors of factor VIIa and thrombin from the Australian sponge Lamellodysidea chlorea
AUTHOR(S): Carroll, Anthony R.; Buchanan, Malcolm S.; Edser, Annette; Hyde, Edward; Simpson, Moana; Quinn, Ronald. J.
CORPORATE SOURCE: Natural Product Discovery, Eskitis Institute, Griffith University, Brisbane, 4111, Australia
SOURCE: Journal of Natural Products (2004), 67(8), 1291-1294
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

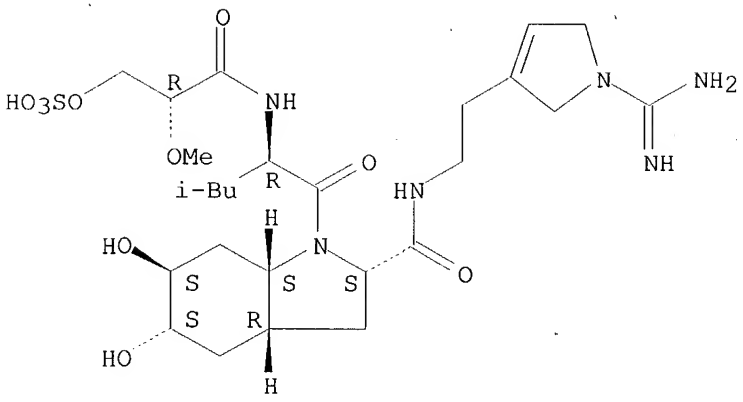
AB Three new marine natural products, dysinosins B-D (e.g. I, dysinosin B), were isolated from the sponge Lamellodysidea chlorea and their structures determined by 1D and 2D NMR spectroscopy. These compds. are inhibitors of the blood coagulation cascade serine proteases factor VIIa and thrombin. These analogs, dysinosins B-D, allowed identification of two structural motifs within the structures that contribute to binding to the proteases, factor VIIa and thrombin.

IT **477708-72-8**, Dysinosin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors of factor VIIa and thrombin from Australian sponge Lamellodysidea chlorea)

RN 477708-72-8 HCAPLUS

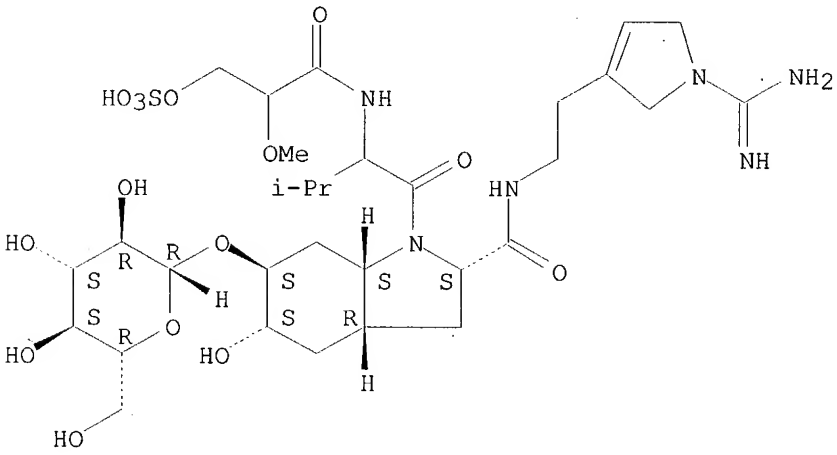
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



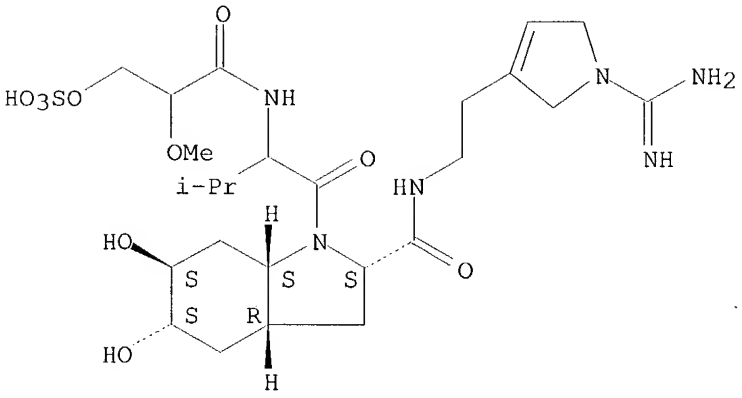
IT **745826-09-9P**, Dysinosin B **745826-10-2P**, Dysinosin C
745826-11-3P, Dysinosin D
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(inhibitors of factor VIIa and thrombin from Australian sponge Lamellodysidea chlorea)
RN 745826-09-9 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Rotation (+).
Currently available stereo shown.



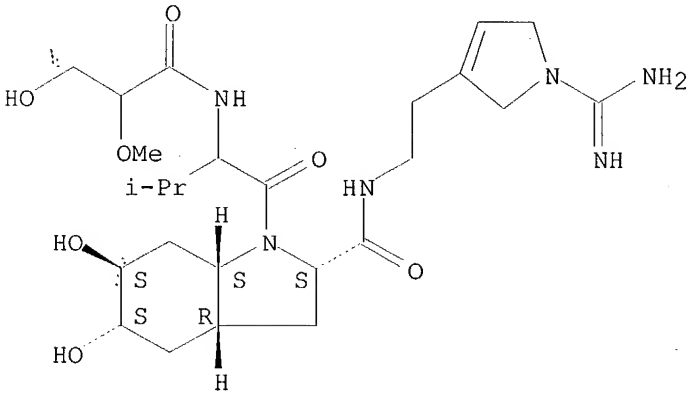
RN 745826-10-2 HCAPLUS
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Currently available stereo shown.



RN 745826-11-3 HCAPLUS
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[(3-hydroxy-2-methoxy-1-oxopropyl)amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Currently available stereo shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:491178 HCAPLUS
DOCUMENT NUMBER: 139:47155
TITLE: Protease inhibitors of the coagulation cascade isolated from dysidea sponges
INVENTOR(S): Goetz, Gilles H.; Harrigan, George G.; Likos, John J.; Kasten, Thomas P.
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051831	A2	20030626	WO 2002-US40001	20021213
WO 2003051831	A3	20031030		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003158248	A1	20030821	US 2002-307803	20021202
US 6716869	B2	20040406		
EP 1465866	A2	20041013	EP 2002-782410	20021213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2004147456	A1	20040729	US 2004-759667	20040116
PRIORITY APPLN. INFO.:			US 2001-341527P	P 20011217
			US 2002-307803	A 20021202
			WO 2002-US40001	W 20021213

AB The present invention is directed toward a composition comprising a compound isolated from Dysidea species sponges that is capable of inhibiting serine proteases of the coagulation cascade. In particular, this composition inhibits the TF/VIIa complex of the coagulation cascade. The invention is also directed toward methods employing this composition as a part of anticoagulant therapy.

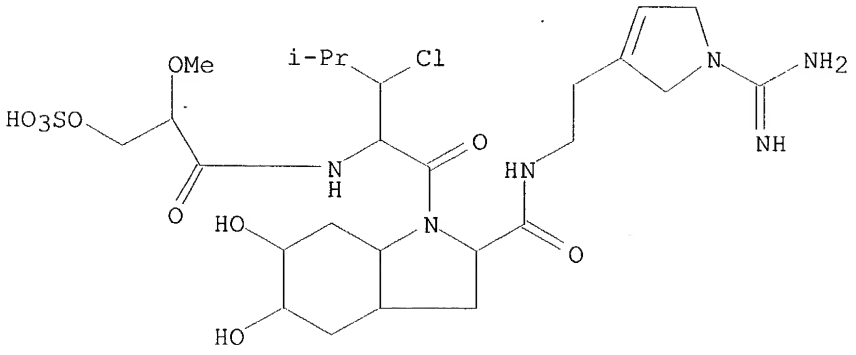
IT **548443-14-7P**

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(protease inhibitors of coagulation cascade isolated from dysidea sponges for anticoagulant therapy in combination with thrombolytic agents)

RN 548443-14-7 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]-1-[3-chloro-2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-dihydroxy- (9CI) (CA INDEX NAME)

Currently available stereo shown.

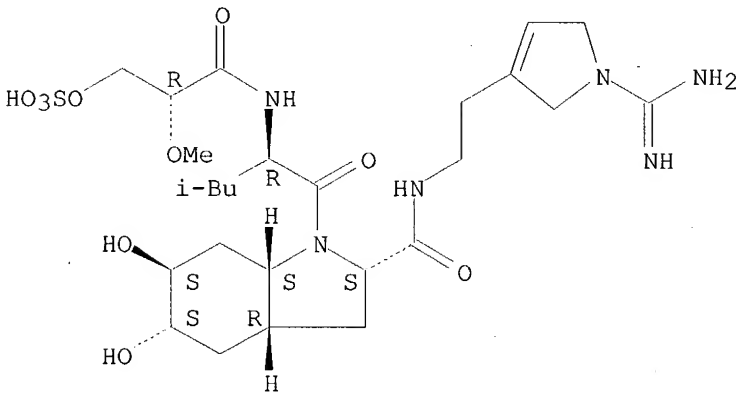


RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(protease inhibitors of coagulation cascade isolated from dysidea sponges for anticoagulant therapy in combination with thrombolytic agents

L6 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:321340 HCAPLUS
DOCUMENT NUMBER: 139:149881
TITLE: New and old challenges in total synthesis. From concept to practice
AUTHOR(S): Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca
CORPORATE SOURCE: Department of Chemistry, Universite de Montreal, Montreal, QC, H3C 3J, Can.
SOURCE: Pure and Applied Chemistry (2003), 75(2-3), 209-221
CODEN: PACHAS; ISSN: 0033-4545
PUBLISHER: International Union of Pure and Applied Chemistry
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. The total synthesis of dysinosin A, a novel member of the aeruginosin group of marine natural products, is discussed. The stereocontrolled synthesis also confirms the proposed structure and absolute stereochem. of the natural product.
IT **477708-72-8P**, Dysinosin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of dysinosin A and confirmation of its structure and stereochem.)
RN 477708-72-8 HCAPLUS
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

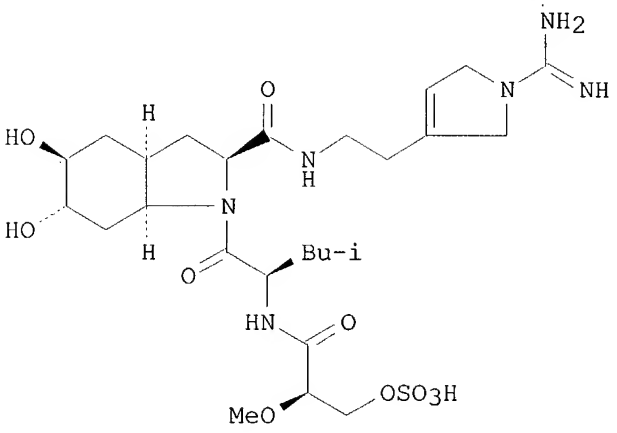
Absolute stereochemistry.



REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:789748 HCAPLUS
DOCUMENT NUMBER: 138:14174
TITLE: Total synthesis and structural confirmation of the marine natural product dysinosin A: a novel inhibitor of thrombin and factor VIIa
AUTHOR(S): Hanessian, Stephen; Margarita, Roberto; Hall, Adrian;

Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca
CORPORATE SOURCE: Department of Chemistry, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
SOURCE: Journal of the American Chemical Society (2002), 124(45), 13342-13343
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:14174
GI



I

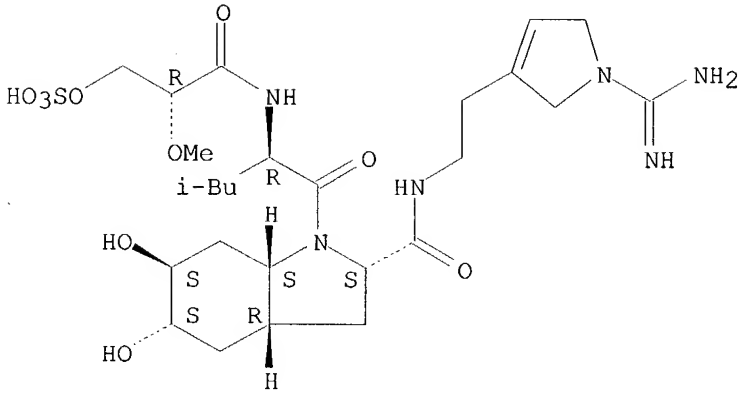
AB The structure and absolute configuration of the marine antithrombotic product dysinosin A (I) was confirmed by total synthesis. The strategy involved disconnection to three subunits, of which two were synthesized from the readily available L-glutamic acid, D-leucine, and D-mannitol. The Grubbs olefin metathesis carbo cyclization reaction was utilized to prepare two intermediates.

IT **477708-72-8P**, Dysinosin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis from amino acids via Grubbs olefin metathesis carbo cyclization of marine natural product dysinosin A, its crystal structure and absolute configuration)

RN 477708-72-8 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

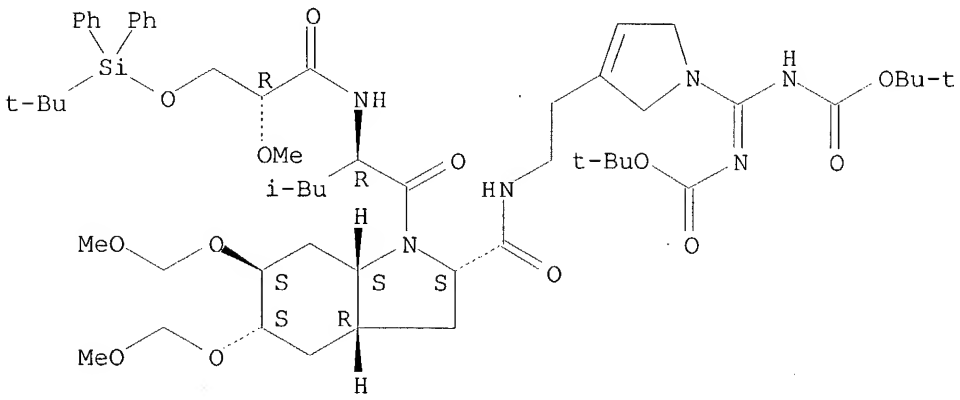
Absolute stereochemistry.



IT **477351-68-1P 477351-69-2P 477351-81-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis from amino acids via Grubbs olefin metathesis carbo cyclization reaction of marine natural product dysinosin A, its crystal structure and absolute configuration)

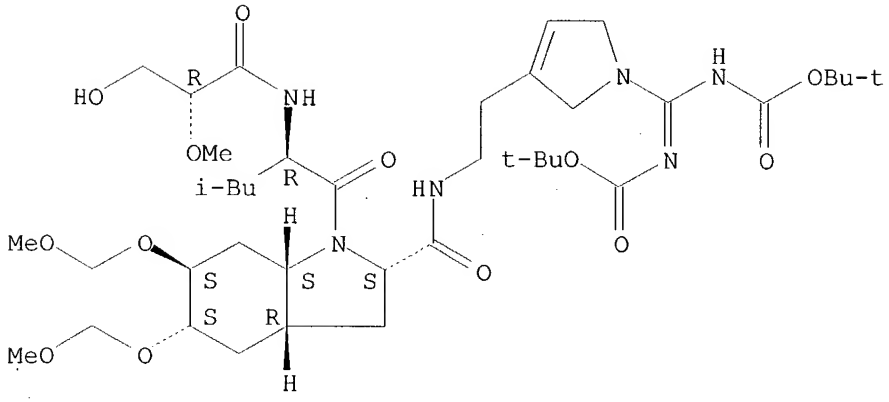
RN 477351-68-1 HCAPLUS
CN Carbamic acid, [[[(1,1-dimethylethoxy)carbonyl]amino][3-[2-[[[(2S,3aR,5S,6S,7aS)-1-[(2R)-2-[[(2R)-3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-2,5-dihydro-1H-pyrrol-1-yl]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



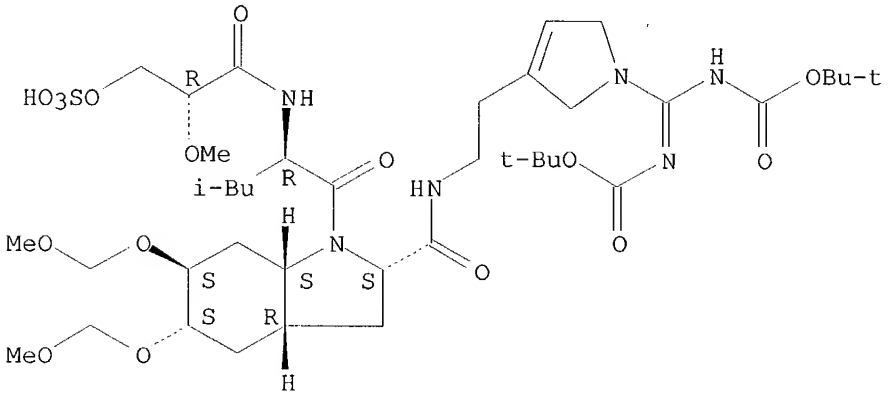
RN 477351-69-2 HCAPLUS
CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-1-[(2R)-2-[[(2R)-3-hydroxy-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-yl][[(1,1-dimethylethoxy)carbonyl]amino]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 477351-81-8 HCAPLUS
CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-5,6-bis(methoxymethoxy)-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-yl][[(1,1-dimethylethoxy)carbonyl]amino]methylene]-, C-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:789746 HCAPLUS
DOCUMENT NUMBER: 138:22307
TITLE: Dysinosin A: A novel inhibitor of factor VIIa and thrombin from a new genus and species of Australian sponge of the family Dysideidae
AUTHOR(S): Carroll, Anthony R.; Pierens, Gregory K.; Fechner, Greg; de Leone, Priscila; Ngo, Anna; Simpson, Moana; Hyde, Edward; Hooper, John N. A.; Bostroem, Stig-Lennart; Musil, Djordje; Quinn, Ronald J.
CORPORATE SOURCE: AstraZeneca R&D, Griffith University, Brisbane, 4111, Australia
SOURCE: Journal of the American Chemical Society (2002), 124(45), 13340-13341

CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

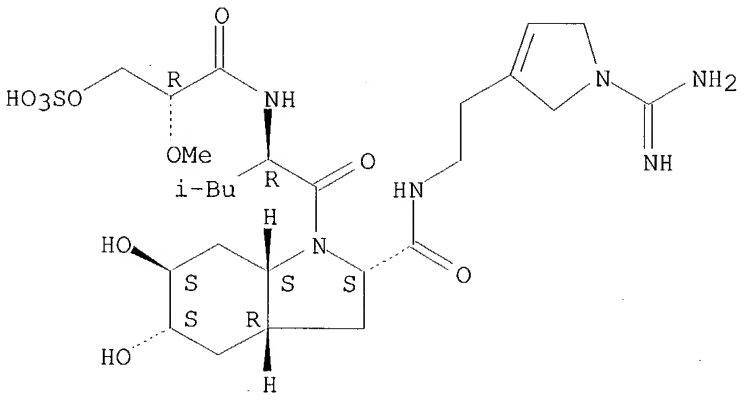
AB A new marine natural product dysinosin A has been isolated from a new genus and species of sponge of the family Dysideidae found near Lizard Island, North Queensland, Australia. Dysinosin A is a potent inhibitor of the blood coagulation cascade factor VIIa and an inhibitor of the serine protease thrombin. Among the distinctive features of dysinosin A are the presence of a 5,6-dihydroxy-octahydroindole-2-carboxylic acid, 3-amino-Et 1-N-amidino-Δ-3-pyrroline, a sulfated glyceric acid, and D-leucine, assembled through three peptidic linkages. Dysinosin A inhibited factor VIIa at a Ki of 108 nM and thrombin at a Ki of 452 nM. The identification of the 1-N-amidino-Δ-3-pyrroline and 5,6-dihydroxy-octahydroindole-2-carboxylic acid as P1 and P2 moieties resp., should pave the way for the design and synthesis of new structure-based inhibitors.

IT **477708-72-8P**, Dysinosin A
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(inhibitor of factor VIIa and thrombin from Australian sponge of family Dysideidae)

RN 477708-72-8 HCAPLUS

CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> fil reg
FILE 'REGISTRY' ENTERED AT 11:28:24 ON 10 NOV 2004
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Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 8 NOV 2004 HIGHEST RN 777024-10-9
DICTIONARY FILE UPDATES: 8 NOV 2004 HIGHEST RN 777024-10-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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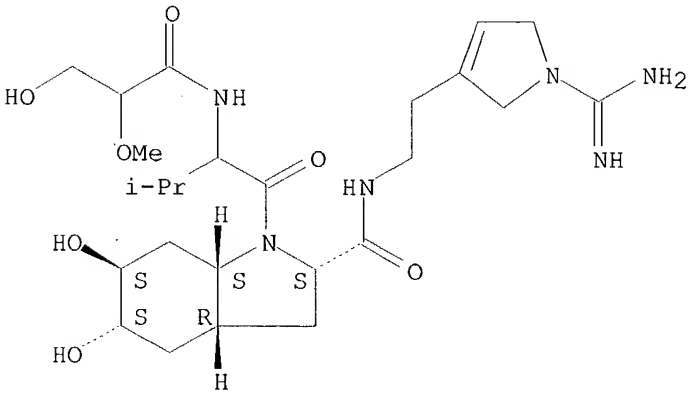
L5 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 745826-11-3 REGISTRY
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[(3-hydroxy-2-methoxy-1-oxopropyl)amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dysinosin D
FS STEREOSEARCH
MF C25 H42 N6 O7
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.
Currently available stereo shown.



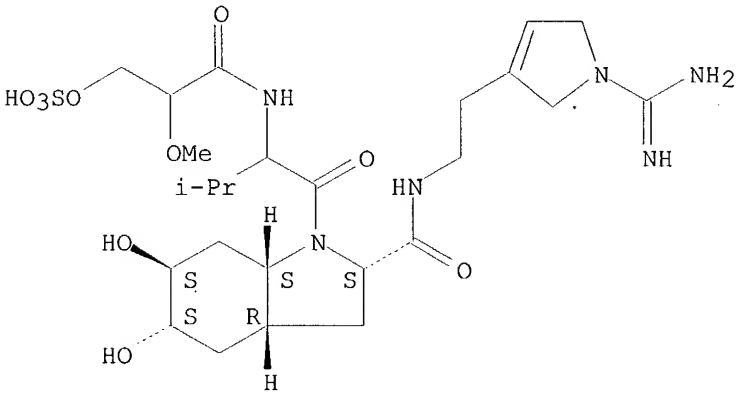
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

L5 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 745826-10-2 REGISTRY
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-3-methyl-1-oxobutyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dysinosin C
FS STEREOSEARCH
MF C25 H42 N6 O10 S
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.
Currently available stereo shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

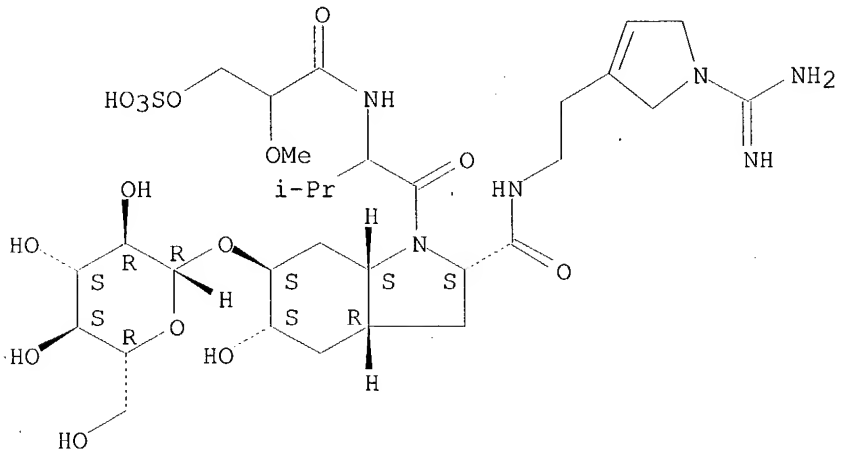
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

L5 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 745826-09-9 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
OTHER NAMES:
CN Dysinosin B
FS STEREOSEARCH
MF C31 H52 N6 O15 S
SR CA

LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties)

Absolute stereochemistry. Rotation (+).
Currently available stereo shown.



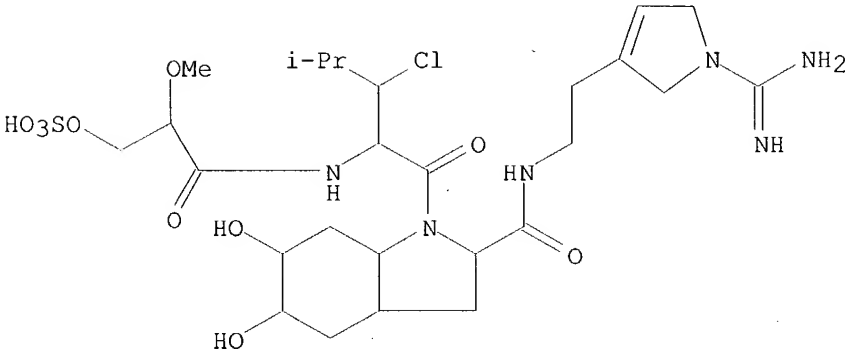
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

L5 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 548443-14-7 REGISTRY
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]-1-[3-chloro-2-[[2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-dihydroxy- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
DR 548443-15-8
MF C26 H43 Cl N6 O10 S
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)

Currently available stereo shown.

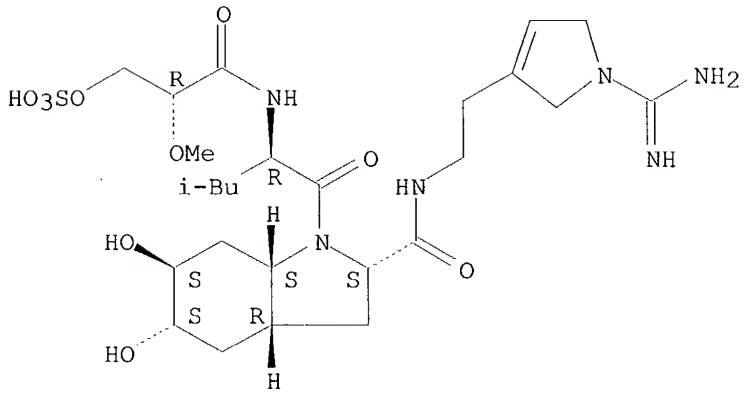


2 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:47155

L5 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 477708-72-8 REGISTRY
CN 1H-Indole-2-carboxamide, N-[2-[1-(aminoiminomethyl)-2,5-dihydro-1H-pyrrol-3-yl]ethyl]octahydro-5,6-dihydroxy-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-, (2S,3aR,5S,6S,7aS)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dysinosin A
FS STEREOSEARCH
MF C26 H44 N6 O10 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, EMBASE, SYNTHLINE
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:221980

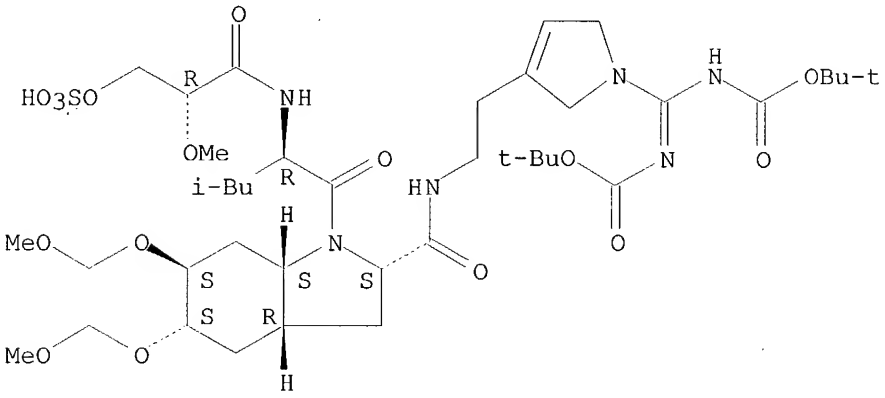
REFERENCE 2: 139:149881

REFERENCE 3: 138:22307

REFERENCE 4: 138:14174

L5 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 477351-81-8 REGISTRY
CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-5,6-bis(methoxymethoxy)-1-[(2R)-2-[[(2R)-2-methoxy-1-oxo-3-(sulfooxy)propyl]amino]-4-methyl-1-oxopentyl]-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-yl][[(1,1-dimethylethoxy)carbonyl]amino]methylene]-, C-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C40 H68 N6 O16 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

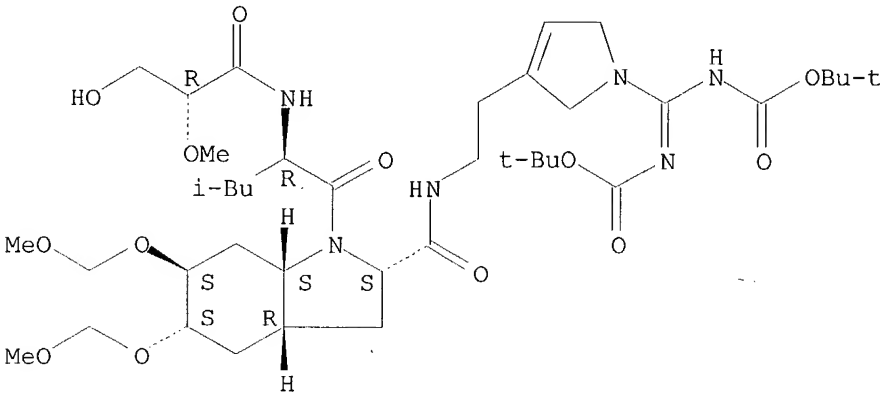
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14174

L5 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 477351-69-2 REGISTRY
CN Carbamic acid, [[2,5-dihydro-3-[2-[[[(2S,3aR,5S,6S,7aS)-octahydro-1-[(2R)-2-[[(2R)-3-hydroxy-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-1H-pyrrol-1-

yl][[(1,1-dimethylethoxy)carbonyl]amino]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C40 H68 N6 O13
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



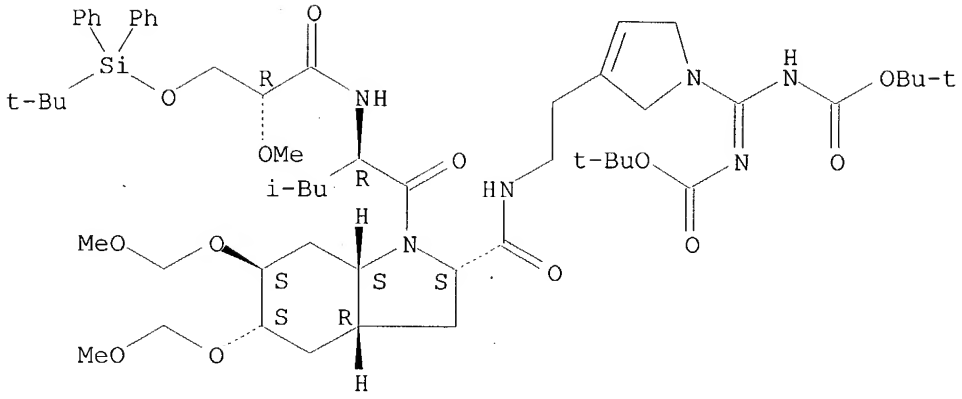
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14174

L5 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2004 ACS on STN
RN 477351-68-1 REGISTRY
CN Carbamic acid, [[[(1,1-dimethylethoxy)carbonyl]amino][3-[2-[[[(2S,3aR,5S,6S,7aS)-1-[(2R)-2-[[(2R)-3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-2-methoxy-1-oxopropyl]amino]-4-methyl-1-oxopentyl]octahydro-5,6-bis(methoxymethoxy)-1H-indol-2-yl]carbonyl]amino]ethyl]-2,5-dihydro-1H-pyrrol-1-yl]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C56 H86 N6 O13 Si
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:14174

=> □

=> fil beil
FILE 'BEILSTEIN' ENTERED AT 11:30:44 ON 10 NOV 2004
COPYRIGHT (c) 2004 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON NOVEMBER 3, 2004

FILE COVERS 1771 TO 2004.
*** FILE CONTAINS 9,073,068 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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*********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.               *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE  *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE         *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                       *
* FOR PRICE INFORMATION SEE HELP COST                               *
*********************************************************************
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NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

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=>
=> d stat que nos
L3              STR
L5            8 SEA FILE=REGISTRY SSS FUL L3
L7            3 SEA FILE=BEILSTEIN SSS FUL L3
L8            3 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L7 NOT L5


=>
=> d brn cn mf fw ctype str rx 1-3


L8   ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

     Beilstein Records (BRN):        9315975
     Molecular Formula (MF):         C40 H68 N6 O16 S . C5 H5 N
     Molecular Weight (MW):          921.07, 79.10
     Compound Type (CTYPE):          heterocyclic

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     FBRN 9314492
     FMF  C40 H68 N6 O16 S
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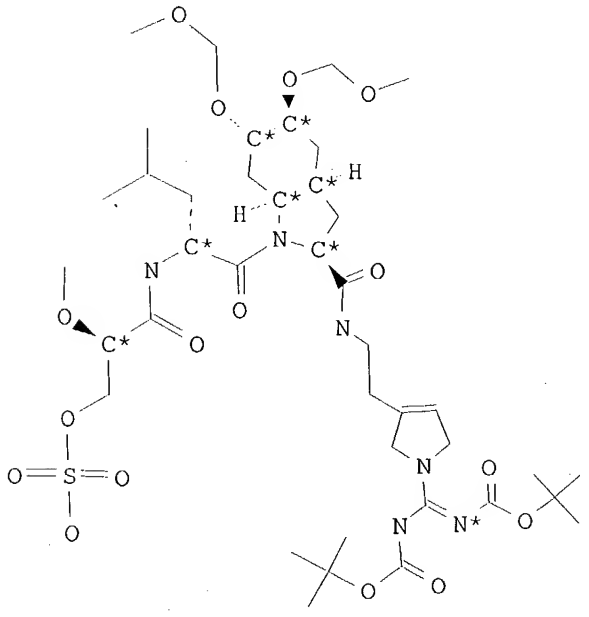

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     CM   2

     FBRN 103233
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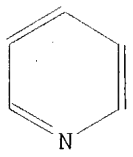
FMF C5 H5 N



Reaction:
RX

Reaction ID (.ID):	9194848
Reactant BRN (.RBRN):	9313827, 3704116
Reactant (.RCT):	(tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester, pyridine; compound with sulfur trioxide
Product BRN (.PBRN):	9315975
Product (.PRO):	C40H68N6O16S*C5H5N
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	9194848.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	dibutyltin oxide
Solvent (.SOL):	CH2Cl2
Time (.TIM):	6 hour(s)

Reference(s):
1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

Reaction:
RX

Reaction ID (.ID):	9232324
Reactant BRN (.RBRN):	9315975
Reactant (.RCT):	C40H68N6O16S*C5H5N
Product BRN (.PBRN):	9311246
Product (.PRO):	dysinosin A
No. of React. Details (.NVAR):	1

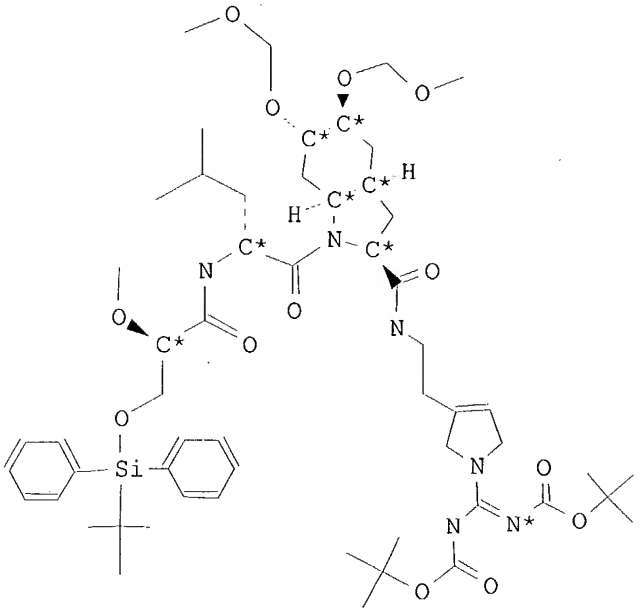
Reaction Details:
RX

Reaction RID (.RID):	9232324.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	TFA
Solvent (.SOL):	CH2Cl2
Time (.TIM):	6 hour(s)

Reference(s):
1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

L8 ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9315558
Molecular Formula (MF):	C56 H86 N6 O13 Si
Molecular Weight (MW):	1079.41
Compound Type (CTYPE):	heterocyclic



Reaction:
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Reaction ID (.ID):	9222715
Reactant BRN (.RBRN):	9311441, 9282636
Reactant (.RCT):	1-<2-<3-(tert-butyl-diphenyl-silanyloxy)-2-methoxy-propionylamino>-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carboxylic acid, <<3-(2-amino-ethyl)-2,5-dihydro-pyrrol-1-yl>-tert-butoxycarbonylimino-methyl>-carbamic acid tert-butyl ester
Product BRN (.PBRN):	9315558
Product (.PRO):	C56H86N6O13Si
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	9222715.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	EDC, HOBt
Solvent (.SOL):	CH2Cl2

Reference(s):

1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT,

124(45), <2002>, 13342 - 13343; BABS-6373650

Reaction:
RX

Reaction ID (.ID):	9232193
Reactant BRN (.RBRN):	9315558
Reactant (.RCT):	C56H86N6O13Si
Product BRN (.PBRN):	9313827
Product (.PRO):	(tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

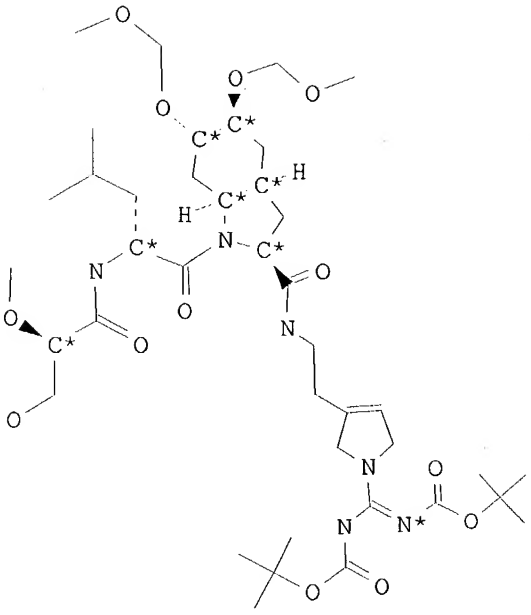
Reaction RID (.RID):	9232193.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	TBAF
Solvent (.SOL):	tetrahydrofuran

Reference(s):

1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

L8 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9313827
Chemical Name (CN):	(tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester
Autonom Name (AUN):	(tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester
Molecular Formula (MF):	C40 H68 N6 O13
Molecular Weight (MW):	841.01
Compound Type (CTYPE):	heterocyclic



Reaction:
RX

Reaction ID (.ID):	9232193
Reactant BRN (.RBRN):	9315558
Reactant (.RCT):	C56H86N6O13Si
Product BRN (.PBRN):	9313827
Product (.PRO):	(tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic acid tert-butyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	9232193.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	TBAF
Solvent (.SOL):	tetrahydrofuran

Reference(s):

1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

Reaction:
RX

Reaction ID (.ID):	9194848
Reactant BRN (.RBRN):	9313827, 3704116
Reactant (.RCT):	(tert-butoxycarbonylimino-<3-<2-(<1-<2-(3-hydroxy-2-methoxy-propionylamino)-4-methyl-pentanoyl>-5,6-bis-methoxymethoxy-octahydro-indole-2-carbonyl>-amino)-ethyl>-2,5-dihydro-pyrrol-1-yl>-methyl)-carbamic

acid tert-butyl ester, pyridine; compound with sulfur trioxide

Product BRN (.PBRN): 9315975
Product (.PRO): C40H68N6O16S*C5H5N
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 9194848.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): dibutyltin oxide
Solvent (.SOL): CH2Cl2
Time (.TIM): 6 hour(s)
Reference(s):
1. Hanessian, Stephen; Margarita, Roberto; Hall, Adrian; Johnstone, Shawn; Tremblay, Martin; Parlanti, Luca, J.Amer.Chem.Soc., CODEN: JACSAT, 124(45), <2002>, 13342 - 13343; BABS-6373650

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